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A new package for simulating periodic boundary conditions in MODFLOW and SEAWAT

V.E.A. Post [1]

VU University, Faculty of Earth and Life Sciences, De Boelelaan 1085, 1081 HV, Amsterdam, The Netherlands

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ABSTRACT

Modeling of coastal groundwater systems is a challenging problem due to their highly dynamic boundary conditions and the coupling between the equations for groundwater flow and solute transport. A growing number of publications on aquifers subject to tides have demonstrated various modeling approaches, ranging from analytical solutions to comprehensive numerical models. The United States Geological Survey code SEAWAT has been a popular choice in studies of this type. Although SEAWAT allows the incorporation of time-variant boundary conditions, the implementation of tidal boundaries is not straightforward, especially when a seepage face develops during falling tide. Here, a new package is presented, called the periodic boundary condition (PBC) package, that can be incorporated into MODFLOW and SEAWAT to overcome the difficulties encountered with tidal boundaries. It dynamically updates the boundary conditions for head and concentration during the simulation depending on a user-defined tidal signal and allows for the development of a seepage face. The package has been verified by comparing it to four different published models of tidally influenced groundwater systems of varying complexity. Excellent agreement was obtained in all cases. The new package is an important extension to the existing capabilities of MODFLOW and SEAWAT with respect to simulating periodic boundary conditions.

1. Introduction

There has been a considerable increase in the number of studies of groundwater systems bordering marine shorelines in recent years. The main impetus for these studies has been the concern over the delivery of terrestrially derived nutrients and contaminants to near-shore coastal waters via subsurface pathways (Slomp and Van Cappellen, 2004; Simmons, 1992), which could adversely affect sensitive marine ecosystems. The outflow of groundwater across the sediment–water interface below the sea floor is commonly denoted as submarine groundwater discharge (SGD). Numerous attempts have been made to quantify the contribution of this process to the water budget of coastal waters, which have relied both on field measurements (e.g., de Sieyes et al., 2008; Burnett et al., 2006; Michael et al., 2003) and modeling (e.g., Li et al., 2009; Robinson et al., 2007b; Li et al., 1999).

In coastal aquifers, groundwater flow patterns and the subsurface salinity distribution are typically influenced by tides (Werner and Lockington, 2006). The propagation of tidal signals in aquifers has been addressed in numerous studies (e.g., Cartwright et al., 2004; Teo et al., 2003; Li et al., 2000; Jiao and Tang, 1999; Nielsen, 1990). Capillary effects may play an important role with the continuous rising and falling of the water table (Li et al., 1997a). More recently, studies have also considered the effect of tidal dynamics on the migration and remediation of contaminants in coastal aquifers (Li and Boufadel, 2010; Robinson et al., 2009; Brovelli et al., 2007; Mao et al., 2006a). These studies have shown that flow geometries due to tidal and variable-density effects result in complex spreading of contaminant plumes and enhanced mixing effects, which tend to promote biodegradation. Further, beach water-table fluctuations have been studied in relation to erosion and offshore sediment transport (Horn, 2006). It has been shown, for example, that there exists a positive correlation between the elevation of the water table and the intensity of beach erosion (Bakhtyar et al., 2009).

One notable aspect of tidal forcing on water table dynamics is the development of a seepage face during ebbing tide (Li et al., 1997b; Turner, 1993). A seepage face is an outcrop of groundwater that develops when the tidal stage drops faster than the water table in the aquifer.

Since coastal groundwater dynamics are controlled by tides, density variations, and unsaturated zone processes, comprehensive models are required to be able to simulate flow and solute transport under these conditions. Analytical solutions have been developed mainly to quantify the propagation into aquifers of tidal

E-mail address: vincent.post@flinders.edu.au
[1] Present address: School of the Environment/National Centre for Groundwater Research and Training, Flinders University, GPO Box 2100, Adelaide, SA 5001, Australia. Tel.: +61 8 8201 5077; fax: +61 8 8201 2676.

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fluctuations and wave run-up below beaches. Several research papers have reported on the use of numerical models of varying complexity (Brovelli et al., 2007; Robinson et al., 2007a, 2007b; Vandenbohede and Lebbe, 2007, 2006; Cartwright et al., 2006). These attempts have demonstrated the challenging nature of the hydraulic modeling of coastal aquifers due to the highly dynamic boundary conditions and the coupling between the equations for groundwater flow and solute transport. Consequently, not all the characteristics of the system under investigation can always be accounted for.

A considerable simplification is to model the saturated domain of the aquifer only, which is appropriate when unsaturated zone processes can be neglected. Under this assumption, it becomes possible to simulate the groundwater system with a variant of the widely used MODFLOW-based codes (Harbaugh et al., 2000). Water table movement is accounted for in MODFLOW by means of a drying–wetting approach. Cells are inactivated when the head becomes lower than the bottom elevation of the cell and become reactivated when the head in a neighboring cell rises above a certain threshold level.

When density effects are negligible, the original MODFLOW code can be used without modification (Kaleris et al., 2002), but coupled groundwater flow and solute transport codes based on MODFLOW exist as well, which allow for simulation of variable-density flow. MOCDENS3D (Oude Essink, 2001) couples MODFLOW to the solute transport simulator MOC3D (Konikow et al., 1996) and has been applied successfully by Vandenbohede and Lebbe (2007, 2006) to model tidal effects on groundwater flow below a sloping beach in Belgium.

SEAWAT (Langevin et al., 2007) combines MODFLOW with MT3DMS (Zheng et al., 1999) and was used by Brovelli et al. (2007) and Robinson et al. (2007a, 2007b) to simulate coastal groundwater dynamics. Although SEAWAT permits the use of time-variant boundary conditions of both head and concentration, the implementation of the dynamic tidal boundary conditions is not trivial (Robinson et al., 2007a). Previous studies have used a two-zone approach in which the ocean domain was explicitly considered in the model and is represented by a series of high-permeability cells in which the tidal signal, imposed at a number of time-variant fixed head cells, propagates rapidly. SEAWAT-based reactive transport models have also been developed (Robinson et al., 2009; Post and Prommer, 2007; Mao et al., 2006b).

In the present paper, a new approach is described that dynamically updates the boundary conditions during a model simulation based on a user-defined tidal signal. It allows for the development of a seepage face and thereby lifts one of the limitations of the original SEAWAT version. Also, input requirements for the model are greatly simplified. Here, the methodology will first be outlined, followed by a set of demonstration examples that show the capabilities of the new code and also serve as verification problems.

2. Approach

The first step in the current approach is to define a series of nodes in the model grid that define the location of the sediment–water, or sediment–air, interface, which will be referred to as interface nodes (Fig. 1). The user chooses these cells based on the locations of their centroids, which should be located at or as close as possible to the interface. Cells that are above the interface are made inactive by the user. Compared to previous SEAWAT-based approaches (Brovelli et al., 2007; Robinson et al., 2007a, 2007b), this reduces the computational demand of the simulations because the zone outside the aquifer is not explicitly represented in the model. It also eliminates the problem of numerical instabilities that are due to the large hydraulic conductivity contrast between the aquifer and surface-water zones (Robinson et al., 2007a).

Under natural conditions, tidal signals can be made up of multiple constituents that act over different time scales. The user-defined tidal level is therefore represented by

$$h_t(t) = h_0 + at + \sum_{i=1}^{n} A_i \cos(\omega_i t - \phi_i), \quad (1)$$

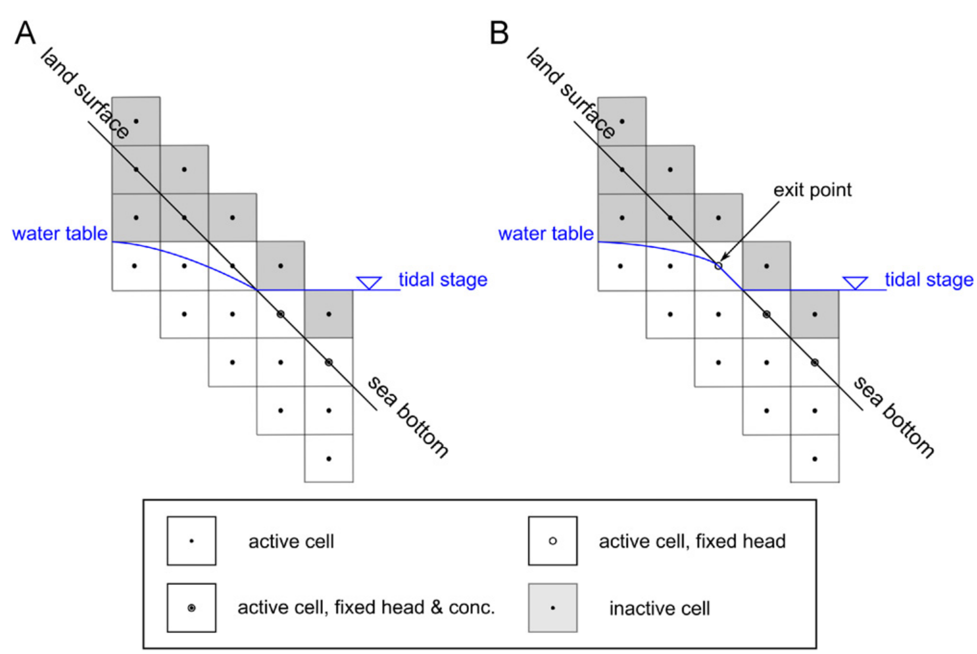

Fig. 1. Boundary conditions at the interface nodes. Interface nodes are the nodes on the diagonal black line representing the land surface/sea bottom. Submerged interface nodes are assigned a fixed head that equals the tidal level and a fixed concentration that equals the surface water concentration. (A) Situation without a seepage face. Exposed interface nodes become inactive if they are dry (i.e., when the head is below the cell bottom). (B) Situation with a seepage face. Exposed interface nodes in cells marked as seepage cells have a fixed head that equals the nodal elevation. Exposed interface nodes that are active always have a variable concentration.